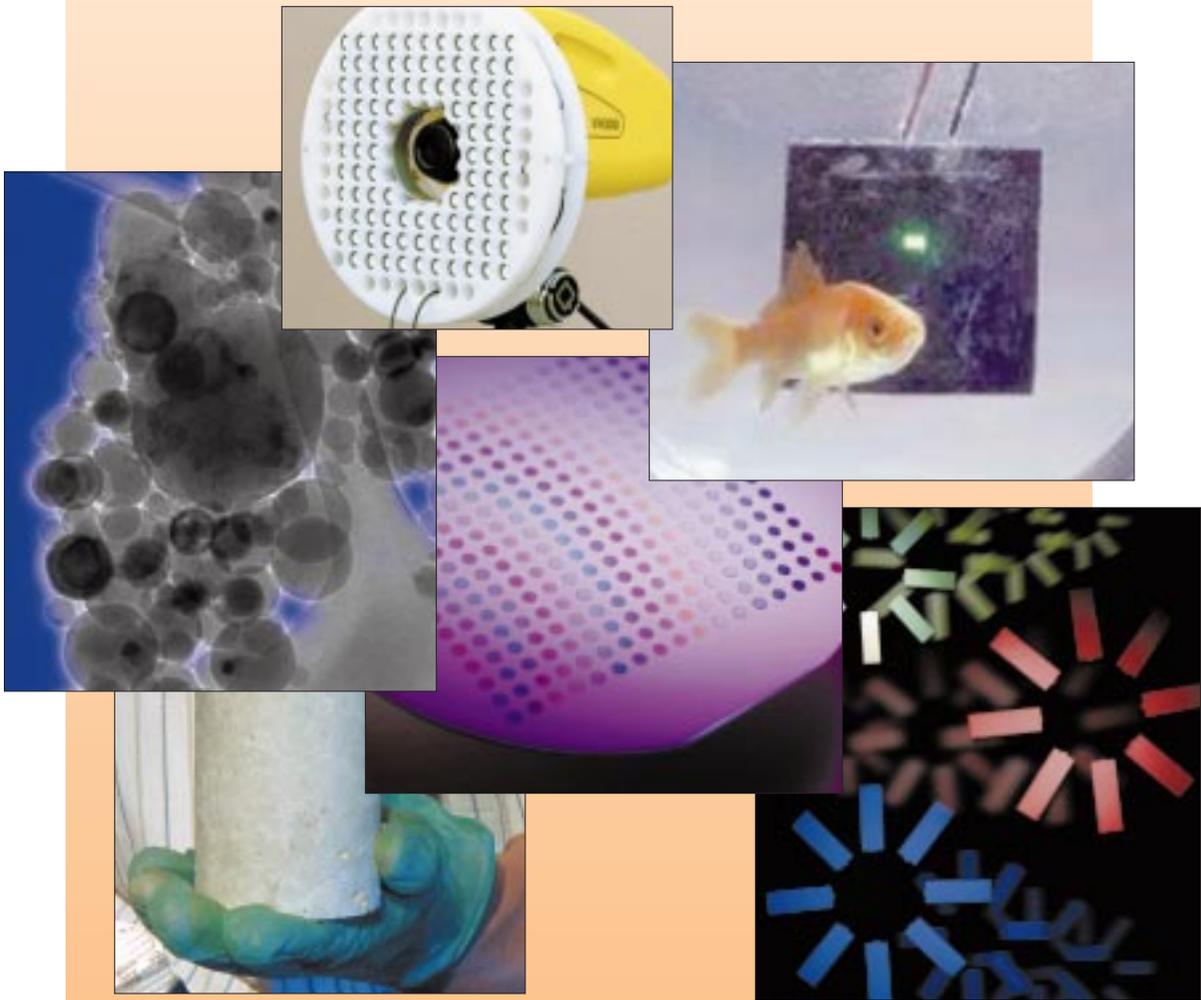


# DATELINE LOS ALAMOS

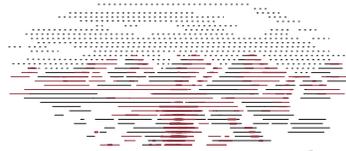
U.S. DEPARTMENT OF ENERGY  
UNIVERSITY OF CALIFORNIA  
SEPTEMBER / OCTOBER 2000



R&D

2000

R&D



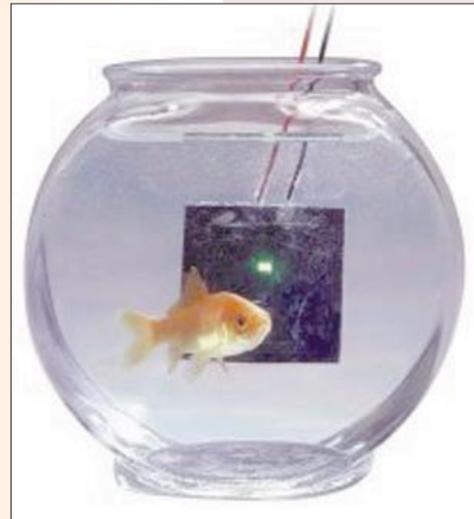
## DATELINE: LOS ALAMOS

### SCIENCE IN THE NATIONAL INTEREST

RESEARCH AND DEVELOPMENT AT THE DEPARTMENT OF ENERGY'S LABORATORIES

America's scientists contribute substantially to the advancement of the nation's science and technology. The Department of Energy laboratories, in particular, help expand the boundaries of basic and applied science and technology with important breakthroughs in energy, materials and chemical science, computing, bioscience and national security. Each year, *R&D Magazine* recognizes a select few of these scientific and technological advances with R&D 100 Awards for the innovations showing the most significant commercial potential.

From televisions to laptop computers, cell phones to digital watches, today's electronic displays are manufactured on glass. As industry strives to improve existing display



technologies and develop a new generation of displays, manufacturers are exploring the use of plastic. Plastic offers increased ruggedness and flexibility and reduced thickness and weight. The fact that oxygen and water vapor can pass through plastic, however, has been a major roadblock in its use. Two ultra barrier coating products developed at Pacific Northwest National Laboratory, Flexible Glass™ engineered substrates and the Barix™ coating, offer extremely high levels of barrier production that can remove this obstacle and play significant roles in the display industry.



## DATELINE LOS ALAMOS

A MONTHLY PUBLICATION OF THE  
PUBLIC AFFAIRS OFFICE OF  
LOS ALAMOS NATIONAL LABORATORY

LOS ALAMOS NATIONAL LABORATORY, AN  
AFFIRMATIVE ACTION / EQUAL OPPORTUNITY  
EMPLOYER, IS OPERATED BY THE UNIVERSITY  
OF CALIFORNIA FOR THE U.S. DEPARTMENT  
OF ENERGY UNDER CONTRACT  
NO. W-7405-ENG-36

#### EDITOR

Meredith Coonley

#### SENIOR SCIENCE WRITER

Todd Hanson

#### EDITORIAL COORDINATOR

Judith Goldie

E-mail the Dateline staff at: [dateline@lanl.gov](mailto:dateline@lanl.gov)

#### CONTRIBUTING EDITOR

John A. Webster

#### CONTRIBUTING WRITER

Michael Carlson

#### PRINTING COORDINATOR

G.D. Archuleta

Information and photographs contained in this issue were provided by Los Alamos' Computing, Information and Communications Division; Argonne National Laboratory; Brookhaven National Laboratory; Lawrence Berkeley National Laboratory; National Energy Technology Laboratory; Oak Ridge National Laboratory; and Pacific Northwest National Laboratory

LOS ALAMOS NATIONAL LABORATORY  
PUBLIC AFFAIRS OFFICE, MS C177  
LOS ALAMOS, NM 87545



## DATELINE: LOS ALAMOS

This issue of *Dateline: Los Alamos* celebrates the recent winners of the R&D 100 Awards competition from the DOE laboratories and highlights all of the Los Alamos National Laboratory technologies nominated for the award in 2000. The technologies nominated by Los Alamos are outstanding examples of the high quality of research and development conducted here.

The R&D 100 Awards program, now in its 38th year, annually honors the 100 most commercially viable products, materials or processes developed by the international research and development community.

Each year technologies are accepted in open competition and judged, both on technical merit and commercial development potential, by technical experts selected by the Illinois-based *R&D Magazine*. Over the years, the R&D 100 Awards have become one measure of a laboratory's contribution to society.

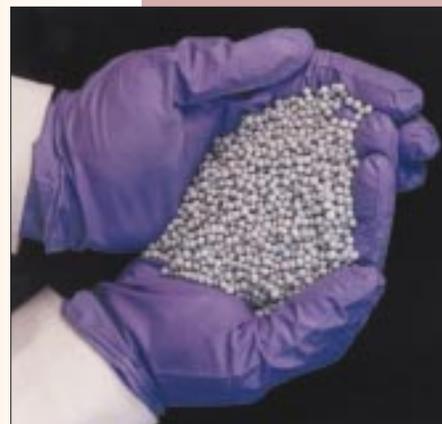
This year, Los Alamos had two award winners, bringing its total to 65 awards over the past 12 years. Quite coincidentally, both of this year's winners are from the Materials Science and Technology Division. Both of the technologies also were developed in collaboration with private-sector companies or with other government agencies, a trend found at other national laboratories.

R&D 100 Award winning technologies are excellent candidates for commercial development. According to Cindy Boone, partnership specialist in Los Alamos' Industrial Business Development Program Office and coordinator of the R&D 100 Awards nomination process for the Laboratory, the majority of Los Alamos' R&D100 Award winners have collaborated with industrial partners to license the technologies and develop commercial applications.

Los Alamos award winner ANDE, an acronym for Advanced Nondestructive Evaluation System, is a detector system that uses ultrasonic interferometry and resonance to rapidly identify the contents of sealed containers.

The ANDE technology was originally developed for the U.S. Defense Threat Reduction Agency for rapid, safe inspection of sealed containers of chemical-warfare compounds and other toxic chemicals during chemical weapons treaty verification. ANDE was a joint entry of Los Alamos and Nick Electronics of Houston. (For more about ANDE, see Page 8.)

Regenerable desulfurization sorbent — RVS-1 — will probably never be a household word, but the cheap, coal-fired electricity made clean by RVS-1 may soon be powering our homes. RVS-1 looks like bunny chow, but acts like a sponge — a remarkably efficient sponge — to remove sulfur from gasified coal used to power turbines that generate electricity. The result? Coal-fired power generation with no sulfur oxide emissions to end up as acid rain. Although the concept of using a sorbent to remove sulfur is not new, what is new about RVS-1 is that it removes nearly all the sulfur, removes it efficiently because it can withstand the high temperatures of gasification, and can be used over and over again, say its developers at the National Energy Technology Laboratory. All that at a cost up to 50 times less than competing products.





## DATELINE: LOS ALAMOS

Another Los Alamos scientist won an R&D 100 Award for helping develop a novel method for creating nanoscale metal powders — powders one-billionth of a meter in diameter — that significantly enhance the effectiveness of rocket fuels and improve lubricants, wear-resistant coatings and batteries.

The electroexploded metal nanoparticles process was originally developed in Russia and refined for peaceful commercial applications in a Los Alamos collaboration with Argonide Corp. of Sanford, Fla.; the National Renewable Energy Laboratory of Golden, Colo.; and the Republican Engineering Technical Center in Tomsk, Russia, through the Department of Energy's Initiatives for Proliferation Prevention Program. (For more on this technology, see Page 10.)

Another example of how national laboratories work with private-sector scientists to achieve award-winning results comes from Lawrence Berkeley National Laboratory.

One of Lawrence Berkeley's two R&D 100 winners this year was combinatorial synthesis, a revolutionary approach to materials research that dramatically accelerates the new materials discovery process by allowing the synthesis of thousands of different chemical compounds on a single substrate.

Using high-throughput testing and structural analysis and characterization of promising materials, the novel method can be used to create and test new materials at rates up to 100,000 times faster than possible using a conventional "small batch" approach.

Symyx Technologies Inc. of Santa Clara, Calif., and Lawrence Berkeley nominated combinatorial synthesis jointly for an R&D 100 Award. By means of an exclusive license agreement granted by Berkeley, Symyx is commercializing the technology through research collaborations.

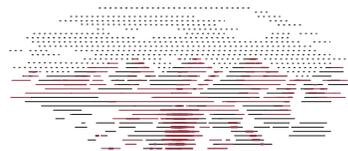
With contributions from a scientist at Lawrence Berkeley, Argonne National Laboratory won an R&D 100 Award for its innovative hard X-ray scanning microprobe. The noninvasive tool focuses X-rays to less than a micron, a scale 1,000 times smaller than traditional X-rays.

With a spatial resolution previously unattainable in X-rays, the technology has the potential to expand the use of traditional X-ray

A patented array for high-throughput screening of new materials is part of combinatorial synthesis —



a revolutionary approach to materials research that dramatically accelerates the discovery of new materials having specific target properties. The technology makes use of rapid simultaneous or parallel synthesis of thousands of different chemical compositions on a single substrate, followed by high-throughput testing and, finally, structural analysis and characterization of promising materials. Novel methods are used to create and test materials at rates up to 100,000 times faster than possible using a conventional "small batch" approach. The underlying principle of the discovery process is to synthesize microscale quantities of thousands of compounds, and then to test these thousands of compounds quickly and reliably. The technology won an award for Lawrence Berkeley National Laboratory and Symyx Technologies Inc.



## DATELINE: LOS ALAMOS

techniques by allowing scientists to study samples without having to specially prepare them.

Biological cells and bacteria, for example, can be examined in their natural state, thereby avoiding problems associated with staining, drying and chemically preparing samples.

The hard X-ray scanning microprobe also can be used to measure structural strains in materials and microelectronic devices, for studying infectious diseases, or for developing smaller, more reliable integrated circuits. The hard X-ray scanning microprobe was one of three R&D 100 Awards received by Argonne this year.

Oak Ridge National Laboratory received three R&D 100 Awards this year and all were developed or submitted jointly with private-sector scientists.

Developed and submitted jointly with Beamline Technology Corp. of Tucson, Ariz., the differentially deposited X-ray microfocusing mirrors technology is an X-ray microscope that gives scientists a powerful new tool for studying materials made up of small disoriented crystal blocks called grains.

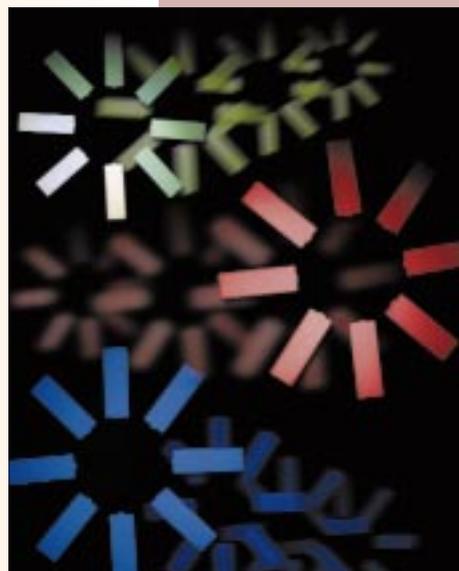
Like the hard X-ray scanning microprobe developed by Argonne National Laboratory, the X-ray crystal microscope provides an exciting capability that didn't exist before, allowing researchers to see the three-dimensional crystal structure of many materials for the first time.

Another Oak Ridge R&D 100 Award winner is high-thermal-conductivity graphite foam. A joint entry with Poco Graphite of Decatur, Texas, the graphite foam has the thermal conductivity equivalent of aluminum with one-fifth its weight. Unlike other carbon foam products, which act as insulators, the nearly 100-percent graphite, open-cell structure material conducts or removes heat.

Because of its superior heat-transfer characteristics, the material could displace heavy cooling fans, metallic fins and heat sinks in electronics and even alter the design of vehicles by allowing radiators to be placed somewhere other than a vehicle's front end.

The Block II chemical biological mass spectrometer developed by Oak Ridge is a joint entry with Orbital

Pacific Northwest National Laboratory's Sunna Dosimeter™ is a small, plastic wafer that is being marketed to accompany food products during irradiation (cold pasteurization). The dosimeter ensures that products receive doses within regulatory requirements. Shining blue light on the irradiated dosimeter induces it to emit red light (fluorescence). The intensity of the red shows the dose value that the food received, with a high degree of accuracy. Cold pasteurization destroys pathogens like E. coli and Listeria. Cold-pasteurized hamburger and chicken, as well as some produce, will be available in a limited number of supermarkets soon, and are expected to be readily available to consumers in the next few years.





## DATELINE: LOS ALAMOS

Sciences Corp. of Pomona, Calif.; MSP Corp. of Minneapolis; Colorado School of Mines in Golden, Colo.; and the U.S. Army Soldier and Biological Chemical Command, Aberdeen Proving Ground, Md.

The Block II is an integrated instrument capable of detecting and identifying both chemical warfare agents and biological warfare agents. It combines the detection speed, sensitivity and specificity necessary for environmental detection of highly diverse classes of materials in a package that is field-portable. Potential primary applications will be on the battlefield with future applications likely to support efforts in counterterrorism, domestic preparedness, law enforcement and health care.

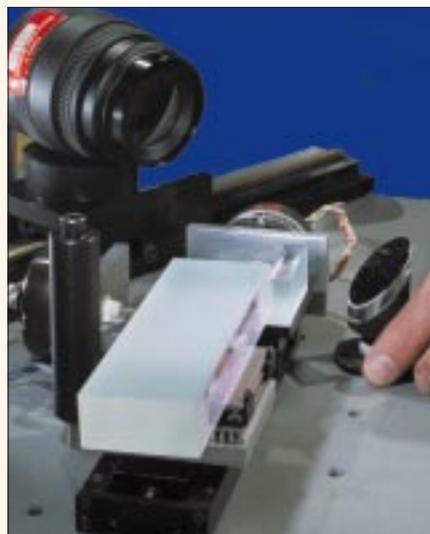
Of course, not all R&D 100 Awards received by DOE national laboratories this year were for joint entries. Many of the winners and R&D 100 entries not mentioned here were the work of single institutions and even single scientists. Scientists at the National Energy Technology Laboratory, for example, have developed a product called RVS-1: the regenerable desulfurization sorbent.

RVS-1 acts like a remarkably efficient sponge to remove sulfur from the gasified coal widely used by power turbines that generate electricity. RVS-1 allows electric power companies to continue or even expand coal-fired power generation by preventing sulfur oxide emissions.

Sulfur oxides can produce acid rain. RVS-1 efficiently removes nearly all the sulfur from gasified coal at a cost up to 50 times less than competing products. The National Energy Technology Laboratory has licensed the exclusive right to produce RVS-1 to Süd Chemie (formerly United Catalysts Inc.) of Louisville, Ky.

Another winning technology comes from Pacific Northwest National Laboratory. The Sunna Dosimeter™ is a small, plastic wafer that can be used to ensure food products receive doses within the regulatory limits during the cold pasteurization (irradiation) process. Cold pasteurized food is likely to be available in a limited number of supermarkets in the near future. The cold pasteurization process destroys pathogens like *E. coli* and *Listeria*.

In another area related to food quality, Pacific Northwest's multi-blade knife failure detector instantly detects knife failures in food processing



The differentially deposited X-ray microfocusing mirror gives scientists a powerful new tool to study interconnects and materials made up of small, disoriented crystal blocks called grains. The new X-ray crystal microscope allows researchers to see the three-dimensional crystal structure of most materials for the first time. It was developed jointly by Oak Ridge National Laboratory and Beamline Technology Inc.



## DATELINE: LOS ALAMOS

lines and triggers the redirection of product flow. Using passive acoustic technologies coupled with special signal discrimination software, the process significantly reduces the amount of food that would normally go to waste after the discovery of a knife break by food inspectors.

The multi-blade knife failure detector is the result of a Pacific Northwest and Lamb-Weston Technical Research Center, Richland, Wash., collaboration. Pacific Northwest also is the winner for an innovative new barrier coating for flat panel displays.

ThermaLock high-performance cement is an innovative material developed by scientists at Brookhaven National Laboratory, Halliburton Company of Dallas and Unocal Corporation of El Segundo, Calif., for use in geothermal energy environments where conventional cement deteriorates rapidly because of carbonation. The product can help extend the productive life of energy-producing geothermal wells by a factor of 20 or more.

This year, 11 DOE laboratories — Argonne National Laboratory, Brookhaven National Laboratory, Lawrence Berkeley National Laboratory, Idaho National Engineering and Environmental Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, National Energy Technology Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Sandia National Laboratories — received 21 out of 100 R&D Awards.

The spirit of scientific discovery is alive and well in the national laboratory system as scientists and managers continue to create and encourage outstanding science and technology and conduct research in the national interest.



Geothermal wells pump hot water or steam from the interior of Earth to drive electricity-

generating turbines. In geothermal environments, an abundance of carbon dioxide causes conventional cement to deteriorate rapidly through a chemical process called carbonation. In contrast, ThermaLock high-performance cement extends the life of geothermal wells by blocking this

destructive chemical reaction. ThermaLock cement is being used commercially and the service life of the product is estimated to be about 20 years. In contrast, conventional cements used in geothermal wells severely deteriorate after only one year. The cement is also particularly suited for use in oil and gas wells and for soil remediation. ThermaLock won an R&D 100 Award for Brookhaven National Laboratory in collaboration with Halliburton Co. and Unocal Corp.



## DATELINE: LOS ALAMOS

**100**  
R&D  
2000 WINNER

### ADVANCED NONDESTRUCTIVE EVALUATION SYSTEM

IDENTIFIES CHEMICALS INSIDE SEALED CONTAINERS

A noninvasive technology that identifies chemical warfare agents and other highly toxic chemicals inside sealed containers at distances up to 15 feet and in less than 30 seconds has been recognized as one of the top innovations of the year by *R&D Magazine*. ANDE — Advanced Nondestructive Evaluation System — was a joint entry of Los Alamos and Nick Electronics of Houston.

ANDE can be used one of two ways: If the container is safe to approach, a sensor is attached to the outside wall; if the container is unsafe to approach, a portable array that sends out a sound beam can be set up within 15 feet of the container. The standoff acoustic measurement capability is especially useful when the immediate environment is unsafe — for example, in a radioactive zone or near leaking systems, highly pressurized containers or containers of unstable explosives.

ANDE uses swept-frequency acoustic interferometry, or ultrasonic interferometry, to send sound waves inside a container, which make the contents resonate, or vibrate. The vibrations are detected with a laser vibrometer and analyzed by a hand-held signal-processing unit. Because each chemical produces its own resonance spectrum, the resulting spectrum can be compared against a database of known chemicals and



The ANDE standoff component is shown in operation. A directed sound beam, originating from the array (inset), interrogates one of the containers in the background. The array transmits a high-frequency wave converted to a low-frequency beam, which is localized near the container. The localized, low sound induces structural vibrations within the container. The vibrations (resonance spectrum) are detected with the laser vibrometer and are analyzed by the

hand-held signal-processing unit. The analysis yields physical properties — such as sound speed, sound attenuation, density and viscosity — which, when compared with an extensive database, uniquely identifies the contents of the container.





## DATELINE: LOS ALAMOS

materials to determine the contents. Currently, ANDE's database covers 120 toxic, hazardous and industrial chemicals.

The current ANDE technology was developed for the U.S. Defense Threat Reduction Agency, where the original application was for rapid, safe inspection of sealed containers of chemical-warfare compounds and other toxic chemicals for chemical weapons treaty verification. ANDE also aids in hazardous materials situations, such as identifying hazardous chemicals in unlabeled storage tanks.

With enhancements to the system's capability, ANDE can aid domestic law enforcement as well. For example, at political conventions and other large gatherings ANDE can analyze the contents of suspect containers. It also can detect dissolved material, such as contraband, in industrial liquids for drug interdiction.

ANDE has applications in the biomedical field as well. It has been licensed by Interferometrics of Houston for developing an instrument to noninvasively characterize blood in humans. In addition, the instrument can monitor osteoporosis and arthritis, using sound speed to measure bone porosity.

The petroleum industry is interested in using the technology for downhole measurement of oil as an inexpensive way to determine the volume fraction of crude oil, brine and gas in real time. Several companies are negotiating licensing for use of ANDE technology in the liquid gas industry and in industrial process control. It also can determine the presence of wax deposition inside pipes, which is an expensive problem for the petroleum industry. Early detection of buildup enables remedial measures that are much less expensive than replacement.

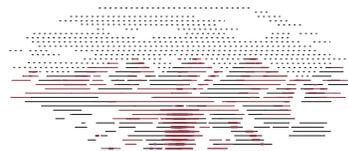
Other applications include determining octane ratings of gasoline, detecting contamination and spoilage of foods — especially dairy and beverages, and detecting wall corrosion inside sealed containers. ANDE can monitor reactor vessels and pipes, and determine liquid-fill levels, even in thick-walled tanks and containers. It also can monitor surfaces such as roads, bridges and airplane wings for ice. At 15 feet the instrument can safely determine the contents and wall integrity of waste storage containers, such as those for the Waste Isolation Pilot Plant in New Mexico. It also can monitor water quality.

The technology underwent two years of extensive field testing and certification by the U.S. Army. The Army has approved it for use on high explosives because of its low-power excitation. The system also has passed all Department of Defense test requirements for DoD field use.

CONTACT: DIPEN SINHA

ELECTRONIC AND ELECTROCHEMICAL MATERIALS AND DEVICES

(505) 667-0062 • [sinha@lanl.gov](mailto:sinha@lanl.gov)



## DATELINE: LOS ALAMOS

**100**  
R&D  
2000 WINNER

### ELECTROEXPLODED METAL NANOPARTICLES

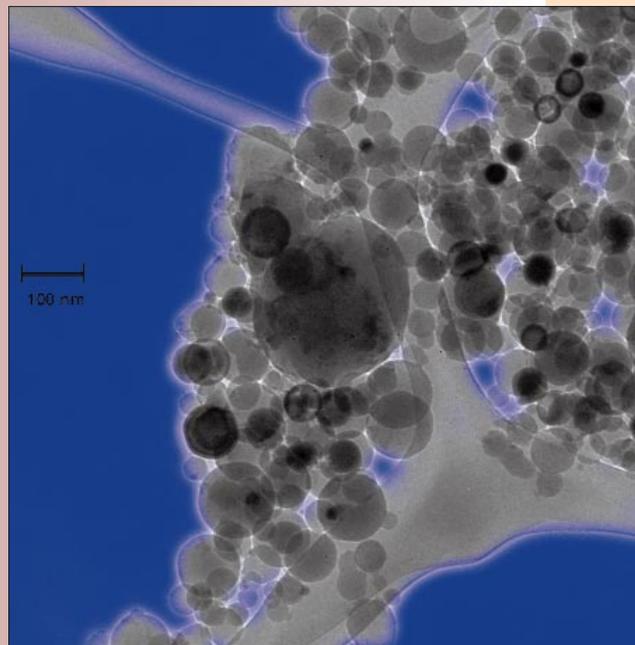
TINY PARTICLES GIVE MORE OOMPF  
TO ROCKET FUELS

Good things come in small packages — or in this case, in small particles. Nanoscale metal powders — powders one one-thousandth of a micron or one-billionth of a meter in diameter — can significantly enhance the effectiveness of rocket fuels as well as improve lubricants, microelectronic circuits, wear-resistant coatings and batteries.

The Electroexploded Metal Nanoparticles technology has earned an R&D 100 Award for Los Alamos; Argonide Corp., Sanford, Fla.; the National Renewable Energy Laboratory, Golden, Colo.; the Department of Energy's Initiatives for Proliferation Prevention Program; and the Republican Engineering Technical Center, Tomsk, Russia.

The nanoparticles are created by passing a large pulse of current through a short segment of fine wire in a controlled atmosphere chamber, creating a metal plasma. The plasma is propelled at supersonic speed through cold gas, which supercools and condenses into particles. Particles are collected in the bottom of the chamber either dry or with a solvent such as kerosene.

The chemical reactivity of a material is related to



This is a high-resolution transmission electron micrograph of Electroexploded Metal Nanoparticles. The chemical reactivity of a material is related to its surface area; the smaller the particle, the greater the surface area per volume. A particle one-tenth the diameter of its larger cousin will have 100 times as much surface area per volume of material.

Electroexploded Metal Nanoparticles can be as much as 500 times smaller, or one ten-thousandth the diameter of a human hair — than the ultrafine metal powders currently available. When they reach this small size their physical and chemical properties change dramatically. The tiny

particles can enhance the effectiveness of rocket fuels as well as improve lubricants, microelectronic circuits, wear-resistant coatings and batteries.



## DATELINE: LOS ALAMOS

its surface area; the smaller the particle, the greater the surface area per volume. A particle one-tenth the diameter of its larger cousin will have 100 times as much surface area per volume of material. Electroexploded Metal Nanoparticles are from 10 to 500 times smaller than the ultrafine metal powders currently available, so their surface area per volume — and reactivity — is immensely greater.

Conventional metal powders are on the micron scale, making it difficult to deposit smooth, dense films because of their large size. Electroexploded Metal Nanoparticles can be as much as 500 times smaller, or approximately one ten-thousandth the diameter of a human hair. The nanoparticles have the potential to revolutionize many applications areas, because when they reach this small a size their physical and chemical properties change dramatically.

Metallic particles have been used to increase the combustion rate of rocket propellants. And because particle size and surface energy is critical, nanoparticles are dramatically superior to micron-sized particles. A higher burning rate increases the thrust that a missile engine can achieve. Metallic nanoparticles also can be used in liquid propellants, such as kerosene. Increasing the volumetric energy density would reduce the tankage weight and overall size of the rocket.

Metallic nanoparticles can be added to organic lubricants to reduce friction and extend the life of heavy-duty engines. They also can be used to make “inks” to “write” on microelectronic circuits and solar cells. Because nanostructures have the promise of substantial increases in hardness and strength, producing inks with single or multiple metals may result in a new class of nanocomposite metal layers.

Another potential application is in batteries: The tiny particles will produce electrodes with higher surface areas, resulting in higher charge and discharge currents and greater cycle life.

Electroexploded Metal Nanoparticles may open up a whole range of new uses for metal powders.

CONTACTS: JOEL KATZ

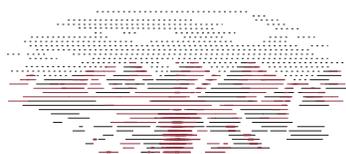
MATERIALS TECHNOLOGY: METALLURGY

(505) 665-1424 • [jdkatz@lanl.gov](mailto:jdkatz@lanl.gov)

FRED TEPPER

ARGONIDE CORP.

(407) 322-2500 • [fred@argonide.com](mailto:fred@argonide.com)



## DATELINE: LOS ALAMOS



The Air-Breather is an efficient, environmentally friendly cylindrical fuel-cell system with no moving parts.

### AIR-BREATHER FUEL CELL STACK FOR PORTABLE POWER APPLICATIONS

The proliferation of portable electronic devices has created a demand for more efficient power sources. Americans purchased and disposed of more than three trillion batteries in 1998. Such a use of resources has prompted the development of a new type of power cell, the Air-Breather. It is compact, reliable, inexpensive, silent, lightweight and environmentally friendly. Lasting at least three times longer than conventional batteries, it produces only water and electricity as byproducts. Multiple Air-Breather units can be networked for larger power needs. Such devices can benefit search-and-rescue operations, police departments, military organizations and others who rely on portable electricity during emergencies. Various industries have expressed interest in this dependable source of electricity for communications, navigation, telemetry and computation in remote or inaccessible locations. Future applications could also include power for cabins, camping, hiking and sailing. The Air-Breather consists of a fuel-cell stack and a small canister that provides hydrogen fuel, which combines with oxygen that diffuses into the stack from the surrounding air. No ancillary devices are used, and there are no moving parts. This was a joint submission of Los Alamos and DCH Technology Inc., Middleton, Wis.

CONTACT: MAHLON S. WILSON  
ELECTRONIC MATERIALS  
AND DEVICE RESEARCH  
(505) 667-9178 • mahlon@lanl.gov

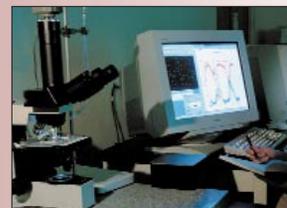
### AUTOMATED VIDEO-MICROSCOPIC IMAGING AND DATA ACQUISITION SYSTEM

Minute particles called colloids are found in everything from airborne smoke and dust to proteins and biological cells. Understanding the behavior of colloids is important in various research fields, including environmental restoration and medicine. The Automated Video-Microscopic Imaging and Data Acquisition System

provides a simpler, cheaper, faster and more precise way to capture and analyze particle motion. The technology combines commercial optical and data-processing equipment with software written to automatically acquire, store, digitize, process, enhance and analyze thousands of colloid images. The system's imaging and data-acquisition components run automatically over long periods, reducing not only the personnel required for experiments but also the potential for human error to invalidate them. The system has been used to study the colloidal transport of waste actinides as part of a Department of Energy project investigating the feasibility of storing nuclear waste in Yucca Mountain Nevada. It can be used to measure the growth kinetics of protein molecules, to study conditions, such as strokes, caused by colloidal transport and to study microorganism deposition on surgical instruments and implants. It also has broad market potential in industries such as papermaking, food and cosmetics, agriculture and water-soluble glues.

CONTACT: AMR ABDEL-FATTAH  
ENVIRONMENTAL TECHNOLOGY  
(505) 272-7195 • amr2450@lanl.gov

A microscope visualizes colloidal particles and the data are extracted and displayed in real time, enabling a user to correct experimental setup errors.



### CHEMICAL DENITRIFICATION PROCESS

Nitrate contamination is a significant health and environmental problem. Excessive nitrate concentrations can destroy life in healthy bodies of water and create "dead zones." The waters of the Mississippi River delta, Adriatic Sea, Baltic Sea, Black Sea and Chesapeake Bay are endangered because of algae growth leading to hypoxia and destruction of marine fauna. Nitrates in drinking water are particularly dangerous to infants and can cause methemoglobinemia, or blue-baby syndrome, which can result in brain damage and death. As the world's population increases, the number of clean drinking-water sources is declining just as the demand for water increases. ChemDen — Chemical Denitrification Process — destroys nitrate contaminants in water



## DATELINE: LOS ALAMOS

by converting them into harmless gaseous nitrogen. The technology is a simple and fast way to ensure a nitrate-free supply of clean drinking water. In the process, sulfamic acid and zinc powder are added to nitrate-bearing waste water. This creates nitrogen gas, which is released into the atmosphere. The acid is completely used in the process and the zinc is recovered and reused. When the reaction is complete, the treated water can safely be released to the environment. ChemDen originally was developed to denitrify



Bubbles of harmless nitrogen gas rise from a beaker containing nitrated waste and enter the atmosphere.

industrial waste water at the Laboratory, but has applications in the steel, fertilizer,

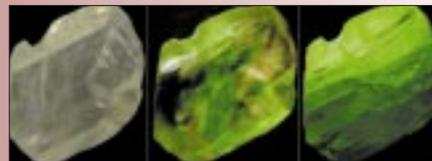
paper and explosives industries and can even be used to eliminate nitrates in agricultural runoff. The technology also can be scaled up or down to fit the need: from huge industrial plant-sized units to smaller units for use by restaurants, hotels, ski resorts, fisheries and small municipalities.

CONTACT: JACEK DZIEWINSKI  
ENVIRONMENTAL TECHNOLOGY  
(505) 667-9792 • jacek@lanl.gov

### DYNAMIC CRYSTALLINE PHASE DETECTION

Determining crystalline phases of materials is crucial in chemistry. A material can exhibit different chemical and physical properties, depending on factors such as temperature and rate of cooling. For example, the common military explosive HMX is stable at its room-temperature phase, but can become unstable and dangerous after being heated. Dynamic Crystalline Phase Detection is a quick, nondestructive tool for determining in situ the crystalline phases of materials based on their optical response to a laser probe. In the case of HMX, it can determine in a split second whether the explosive is safe to handle. The technology uses a commonly available laser and a technique called second harmonic generation, which doubles the frequency of a laser beam as it reflects from a sample material.

Using  
Dynamic  
Crystalline  
Phase  
Detection,  
researchers  
can



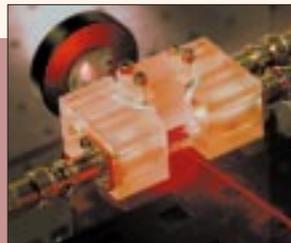
distinguish between different chemical phases quickly by the change in the color of the laser light.

The change in color of the light reflected from the sample material lets researchers distinguish between sensitive and insensitive forms of explosives, for example, and to understand the transformation process between the two forms. DCPD has applications in national security, intelligence and counterterrorism as well as in the commercial explosives industry, which supplies explosives for mining, highway and tunnel construction, and oil and gas exploration. The technique also will be useful in the pharmaceutical industry, giving researchers a fast way to determine the rate of dissolution, rate of crystallization and purity of drugs.

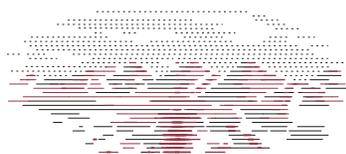
CONTACT: BLAINE ASAY  
HIGH EXPLOSIVE SCIENCE  
AND TECHNOLOGY  
(505) 667-3266 • bwa@lanl.gov

### INTEGRATED FOCUSING SCANNER

Laser-beam scanning and focusing are essential functions for optical communications, data storage, printing and scanning. These technologies form the basis for the everyday tasks of our modern information infrastructure. The Integrated Focusing Scanner — INFOSCAN — combines a dynamic, variable-power focusing lens and a large-angle laser-beam scanner into a single, integrated optical device. The dynamic lens permits adaptable focusing of light to or from an optical fiber or optical storage medium while the beam scanner deflects the beam over a continuous large angle — all in a compact, energy-efficient package with no moving parts. The INFOSCAN functions by applying electric fields across a thin



The INFOSCAN in operation. The actual device is the thin wafer mounted in a plexiglass test block from which the laser beam emanates.



## DATELINE: LOS ALAMOS

ferroelectric wafer in which microdomains in the shape of optical components have been patterned. INFOSCAN's quick read/write capability and variable focusing may enable faster, more reliable Internet connections and data storage. It also will benefit military and space needs by providing rapid laser scanning capability for communications and target tracking, as well as more mundane technologies such as grocery store checkout scanning and laser-light entertainment and displays. It may even provide doctors with more accurate assessments of patient health by improving laser-based scanning diagnostics and treatment, such as the detection of cancers and blood monitoring, and enhance treatment options such as retinal surgery and laser vision correction. Virtually any optical device that incorporates a lens and beam deflector may benefit from the increased flexibility, speed and stability of the INFOSCAN. The technology was developed in collaboration with Los Alamos and Pennsylvania State University.

CONTACT: KEVIN GAHAGAN  
PHYSICAL CHEMISTRY  
AND APPLIED SPECTROSCOPY  
(505) 667-6281 • ktg@lanl.gov

LA-MAP's miniature  
microwave-plasma torch.



### LOS ALAMOS MONITOR FOR AIR PARTICULATES

The Occupational Safety and Health Act, passed in 1970, ensures Americans the right to safe and healthful working conditions, but workplace hazards continue to inflict a toll in both human and economic costs. For example, occupational exposures to some airborne particulates are known to cause chronic obstructive pulmonary diseases, including asthma. Reliable ways to quickly assess exposures are critical to managing the risk and preventing illness and injury. The one-of-a-kind portable Los Alamos Monitor for Air Particulates — LA-MAP — identifies in real time all hazardous elements of the periodic table, both metal and nonmetal. The invention is unique in its ability to tell workers immediately if an industrial operation is exceeding air-particulate standards. LA-MAP includes a microwave-plasma

source, optical-beam collection assembly, optical-beam dispersal device and a signal detector. In addition, it contains an in situ air-particulate sampling system and a computer-controlled data-processing system, all within the dimension of a computer monitor and weighing only about 55 pounds. The instrument initially was developed to address the critical problem of chronic beryllium disease in the Department of Energy's nuclear weapons complex. Worker exposure to beryllium, a very strong yet lightweight metal essential to nuclear weapons, has caused debilitating health problems, and the metal also is used in the manufacture of missiles, aircraft, satellites, automobiles, home tools, computers, golf clubs and bicycles. LA-MAP could become a fundamental tool for monitoring air pollution, hazardous dust caused by mining and other industrial processes including automobile-engine testing facilities, construction sites and welding.

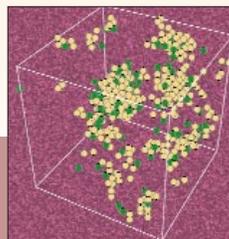
CONTACT: YIXIANG DUAN  
ANALYTICAL CHEMISTRY SCIENCES  
(505) 665-9219 • yduan@lanl.gov

### MOLECULAR DYNAMICS

#### LATTICE GAS

How did nonliving matter become living matter? A new simulation method — Molecular Dynamics Lattice Gas — offers unique computational capabilities for studying the complex molecular interactions and chemical reactions that scientists believe created life eons ago on Earth as well as on other planets. The origin of life is to a great extent a historical question, which we will probably never be able to answer in detail. Thus, the focus is on modeling the simplest, thermodynamic downhill process that bridges this gap using the same materials presumably available when Earth was formed. Defining these steps requires a detailed understanding of molecular self-assembly and self-organization processes that cannot be provided by conventional computer simulations because of their time and length scales. Besides aiding scientists in their quest to recreate life in the

laboratory, MD lattice gas can be used to support a variety of basic and applied research applications.



An MD lattice gas simulation of a micelle formation in an aqueous environment.



## DATELINE: LOS ALAMOS

Many new materials being developed are composed of multiple layers of self-assembled polymers, such as the biomimetic membranes used for sensors. MD lattice gas can simulate the assembly of these multilayer membranes better than traditional techniques. Because biomedical applications involve membrane interactions with other molecules, MD lattice gas simulations can be used in gene therapy to study the diffusion of DNA across a membrane. The simulation also has applications in the oil and gas industry, where it can be used to determine what effect pumping in detergents or additional water will have on oil recovery or give details of the mineral, water and hydrocarbon interactions within oil-bearing rock. MD lattice gas simulations also can be used to study details of subsurface plutonium transport to assess the viability of storing radioactive nuclear waste at geologic repositories such as Yucca Mountain, Nevada.

CONTACT: STEEN RASMUSSEN  
GEOANALYSIS  
(505) 665-0052 • steen@lanl.gov

With OpenEMed, an authorized physician can view a computerized patient medical record that includes data retrieved over the Internet from data repositories at widely separated facilities.



### OPENEMED — VIRTUAL MEDICAL RECORD SYSTEM

Reviewing the growing volume of paper patient records can overwhelm physicians and significantly reduce one-on-one time between doctor and patient. The Internet-based OpenEMed software gives physicians a secure electronic medical record that integrates treatment history, test results, prescriptions, immunization records and radiological images on a single computer screen. It integrates information from separate — even geographically separate — repositories. OpenEMed is a suite of standard components that securely communicate over the Internet: the application on the user's computer, an authentication server that admits only authorized users and verifies their need-to-know access, an identification server that

identifies patients and a clinical observation access service that retrieves requested clinical data. The components are written in the Java programming language, allowing OpenEMed to be run on any platform. OpenEMed can use multiple databases, regardless of their originating platform or architecture. It also can be integrated with systems that implement the same standard interfaces. Besides helping physicians manage patients' healthcare, OpenEMed can be used to conduct remote medical consultations between primary-care physicians and specialists, track immunizations, manage clinical trials on new pharmaceuticals, track diseases while preserving patient anonymity and compile case studies for use in medical training.

CONTACT: DAVID FORSLUND  
ADVANCED COMPUTING LABORATORY  
(505) 665-1907 • dwf@lanl.gov

### OPTICAL PHARMACOKINETICS SYSTEM

The rising cost of pharmaceutical research and development has limited the availability of next-generation drugs such as chemotherapy drugs and photodynamic therapy agents. Photodynamic therapy is a relatively new cancer treatment in which an agent that localizes in cancer tissues is activated by light to cause cell death. The average cost of developing a new drug from concept stage is \$300 million to \$600 million. High development costs are passed on to insurance companies, who in turn attempt to control costs by limiting coverage. Thus, potentially life-saving drugs are not always available to people who need them. The Optical Pharmacokinetics System promises to reduce the costs of pharmaceutical R&D for some drugs by streamlining experiments. The system's easy-to-use instrumentation allows real-time in vivo measurements of drug concentrations at specific tissue sites, making it possible to determine the complete pharmacokinetics for a given drug dosage at specific tissue sites of an organism. The tip of a probe is placed in gentle contact with the surface of the tissue sites being studied. Light enters the tissue from one of the two fibers in the probe and is collected by the second fiber for analysis.

The Optical Pharmacokinetics System makes noninvasive measurements of drug concentrations in tissue.



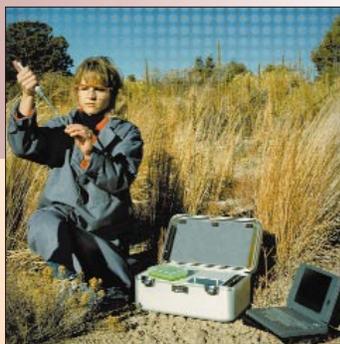


## DATELINE: LOS ALAMOS

to determine the drug concentration at that specific site. Each measurement takes less than one second. The optical pharmacokinetics system shows promise for additional application as well, such as measuring blood pooling in tissue and monitoring oxygenation, both important in determining the response to chemotherapy treatment. The project is a collaboration between Los Alamos, University of California, San Diego and other universities.

CONTACT: IRVING J. BIGIO  
BIOSCIENCE DIVISION  
(505) 667-7748 • [ijb@lanl.gov](mailto:ijb@lanl.gov)

The PDQ can be used in the field to measure DNA in an environmental sample.



### PORTABLE DNA QUANTIFIER

Obtaining reliable and quantitative DNA from soil samples is often a difficult task for scientists in the field. Crude DNA must be purified before it is quantified, and often the minute amounts of DNA collected prohibits technicians from performing an accurate analysis. Furthermore, researchers must often send samples to distant laboratories for laborious and time-consuming testing methods. The Portable DNA Quantifier for Environmental Analysis can rapidly and accurately quantify small amounts of DNA in soil and biological samples despite the presence of interfering contaminants. With incorporated software, an operator is directed through the sample preparation process, ensuring an accurate detection and measurement of DNA. Investigators can use the PDQ to assist with instant crime-scene analysis of blood, semen, bone and other DNA sources. It can also be used with other equipment to aid in the detection of biological warfare agents at suspicious facilities. The PDQ can function as a multipurpose aid for university laboratories, and accompanied by other instruments, assist as a pathogen detector in the agriculture and food industries where bacteria such as *E. coli* are common. With the PDQ, results are

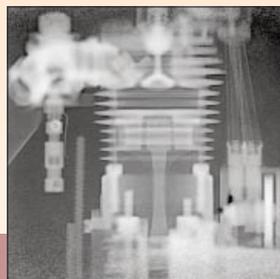
precise and easily understood. Chain-of-custody issues related to crime-scene evidence are eliminated. The technology was developed with Opti-Sciences Inc. of Tyngsboro, Mass.

CONTACT: PETER C. STARK  
APPLIED CHEMICAL TECHNOLOGY  
(505) 667-0724 • [pstark@lanl.gov](mailto:pstark@lanl.gov)

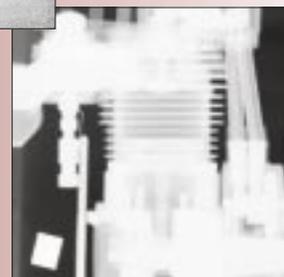
### PROTON RADIOGRAPHY

The ability to nondestructively penetrate solid objects to reveal their internal structure has been widely used since the discovery of X-rays more than a hundred years ago. X-ray imaging has had major impacts on science, technology, medicine and industry. Proton radiography possesses an even greater ability to reveal the internal structure of an object. Protons were first used to make low-dose medical radiographs nearly 30 years ago, but those early proton radiographs suffered from blurring. Recently, however, researchers have developed an innovative Zumbro lens that greatly reduces image blurring and allows a resolution about 10 times greater than that possible with intense pulsed X-ray machines. Besides improving the quality of low proton dose medical X-rays, proton radiography can produce images of shock fronts and combustion waves within metal containers and identify the individual parts in complex objects such as engines and weapons systems. The technology also can be used to produce radiographic movies whose total frame numbers are limited only by the number of cameras used. Hundreds or thousands of frames per movie eventually will be

possible as well as high-quality three-dimensional tomography movies. These movies can be used to study the performance of internal combustion engines, jet



A model airplane engine and radiographs of it produced by 800-million-electron-volt protons (top) and about 100,000-electron-volt X-rays.





## DATELINE: LOS ALAMOS

turbines, high explosives and nuclear weapons. The technology was a joint submission of Los Alamos and Bechtel Nevada.

CONTACTS: CHRIS MORRIS  
SUBATOMIC PHYSICS  
(505) 667-5652 • cmorris@lanl.gov  
RICHARD THOMPSON JR.  
BECHTEL NEVADA  
(505) 663-2115 • thompsrt@lanl.gov

### QTL BIOSENSORS

A novel biosensor is a breakthrough tool based on a new science. The quencher-tether ligand luminescent biosensor detects biological molecules through a quenched-fluorescence-recovery approach. The high sensitivity of certain fluorescent polymers to quenching — being extinguished — is a recent discovery and represents a new field of scientific inquiry. This high quenching sensitivity has been captured in the design of the QTL biosensor.



Even with the naked eye, it's evident that the fluorescence in the vial on the left has been extinguished.

The new sensor will be able to identify, in less than 1 second or about 1,000 times faster than other technologies, biological and chemical agents, such as viruses, bacteria, proteins and chemical and biological warfare agents. In addition to sensing and medical diagnostics, it shows tremendous promise for the development of new products for pharmaceutical and biomedical research, and for monitoring biological functions such as immune system response. Researchers are developing a simple-to-operate, inexpensive unit about the size of a hand-held calculator for use in the field. The operator would merely have to inject a quantity of the sample into the device, press a button for instant analysis and check for the absence or presence of fluorescence. By using existing libraries of antigens and antibodies, the QTL biosensor can quickly detect thousands of compounds. New detection combinations also can be designed based on specific requirements.

Because of its portability, robustness, sensitivity and flexibility, the biosensor has the potential to revolutionize biomedical research and open new frontiers in biotechnology and medicine. QTL Biosystems LLC of Santa Fe, N.M., is developing and marketing the detection capabilities of the biosensor.

CONTACTS: DAVID WHITTEN  
BIOSCIENCE DIVISION/QTL BIOSYSTEMS LLC  
(505) 424-1000 • whitten@qtlbio.com  
DUNCAN MCBRANCH  
BIOSCIENCE DIVISION/QTL BIOSYSTEMS LLC  
(505) 424-1000 • mcbranch@qtlbio.com

### RADIATION LITMUS PAPER

The threat of radiation exposure affects the lives of laboratory workers and the general public every day. For example, improperly discarded medical radiation sources have caused serious injuries and deaths when they are found by children who treat these sources as toys. Other radiation sources have been mixed with recycled scrap metal, contaminating recycling facilities and costing millions of dollars to clean up. Current technology is either too expensive for widespread use or does not warn the user quickly enough. Radiation Litmus Paper makes real-time dosimetry cost-effective and easy to use, especially for the occasional user. Radiation Litmus Paper produces a simple color change in response to low doses of ionizing radiation. It is nontoxic and possesses a long shelf life, allowing consumers to use Radiation Litmus Paper immediately without concern about battery life or further calibrations.

CONTACT: BENJAMIN P. WARNER  
CHEMICAL AND ENVIRONMENTAL  
RESEARCH AND DEVELOPMENT  
(505) 665-6962 • warner@lanl.gov

The Radiation Litmus Paper device, slightly larger than a credit card, contains a solution that changes color when the user is exposed to radiation,





## DATELINE: LOS ALAMOS

The Spent Fuel Coincidence Counter is the only nondestructive assay device that measures the plutonium content of spent-fuel assemblies.



### SPENT FUEL COINCIDENCE COUNTER

It's relatively easy to build fences and post security guards to protect sensitive items like nuclear material, but it is much more difficult and more important to know how much nuclear material is actually inside the fence. It is even more difficult to prove that the fence or guards have never been compromised. Because the plutonium generated in breeder reactors is of high-quality weapons grade, breeder-reactor spent fuel is attractive to rogue states or terrorist organizations. The Spent Fuel Coincidence Counter (SFCC) uses a combination of lead shielding and an array of a new type of gamma-insensitive helium-3 tube detectors to detect neutrons coming from spent fuel and determine the mass of plutonium in the spent fuel. It is the only nondestructive assay device of its kind. Chemical analysis produces similar results on a very limited number of items, but it is difficult to perform and expensive. In addition, the process can take up to two weeks. By being able to accurately and quickly measure the total plutonium content of their spent-fuel assemblies, managers of breeder-type nuclear reactors can account for their spent fuel and its plutonium and protect it from being diverted to nonpeaceful purposes. The technology has been used to measure the plutonium content of oxide, mixed-oxide and metal spent fuel. Mixed-oxide fuel already is used in a number of reactor facilities around the world. The SFCC has been used successfully by the International Atomic Energy Agency in Kazakhstan.

CONTACT: PARRISH STAPLES  
SAFEGUARDS SCIENCE AND TECHNOLOGY  
(505) 665-0250 • staples@lanl.gov

### THERMAL IONIZATION CAVITY SOURCE FOR MASS SPECTROMETRY

Thermal ionization mass spectrometry (TIMS) is used to determine both the abundance and the isotopic composition of elements in many

different types of samples. Because thermally generated ion beams are stable and long lived, they permit acquisition of extremely precise data. The technique is highly sensitive, thus data can be acquired from very small samples. However, established TIMS methods can be inefficient and time consuming. The Thermal Ionization Cavity (TIC) Source for Mass Spectrometry enhances TIMS performance and reduces sample preparation and analysis time. Solid or dried solution samples are inserted directly into the TIC, a tungsten wire with a tiny tube-like cavity in one end. The TIC is heated by electron bombardment to greater than 2,500 degrees Centigrade. The closed cylindrical geometry of the TIC source provides greater surface area than that of a filament ion source, thereby enhancing ion production. The TIC source can also withstand greater temperatures than the filament source, thus enhancing ion production further. The TIC is interfaced to a time-of-flight mass spectrometer (TOFMS), and the complete system includes methods for multi-element isotopic analysis, data collection, dedicated software and spreadsheet-compatible data processing. The TIC-TOFMS will be valuable to nonproliferation agencies, forensic scientists and law enforcement agencies faced with having to characterize rapidly and accurately the nature and origin of nuclear and other particles. The present system costs less than \$50,000 to assemble, and its affordability will extend sophisticated analytical methods and technology

to many more users, including small laboratories and universities.

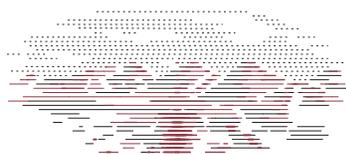


The housing for the TIC source and the interface to the time-of-flight mass spectrometer.

CONTACT: DAVID M. WAYNE  
PIT DISASSEMBLY  
AND SURVEILLANCE TECHNOLOGY  
(505) 665-7552 • d-wayne@lanl.gov

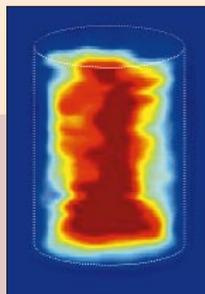
### TOMOGRAPHIC GAMMA SCANNING SYSTEM

Determining the contents of sealed radioactive waste containers is a necessary, costly and sometimes hazardous part of nuclear safeguards and waste management. Tomographic Gamma



## DATELINE: LOS ALAMOS

Scanning (TGS) is a nondestructive assay technique that is being used to safeguard and certify transuranic waste at Rocky Flats, Colo., before it is shipped to the Waste Isolation Pilot Plant in New Mexico. TGS reduces the cost of safeguards and waste characterization by accurately and rapidly measuring gamma-ray-emitting materials inside sealed waste containers as large as 83 gallons. By combining computerized tomography with high-resolution gamma-ray spectroscopy, TGS can assay a wide range of radioisotopes accurately. Because TGS can locate radioisotope deposits inside sealed containers, the expense and hazards associated with repackaging operations is reduced. TGS can be used to screen low-level medical waste or waste from reactor reprocessing facilities and to characterize radioactive tracers in porous media. It also can be used to characterize industrial processes involving radioactive isotopes such as the distribution of fission products in spent fuel. This information could be used to detect missing rods in fuel assemblies at nuclear power plants.

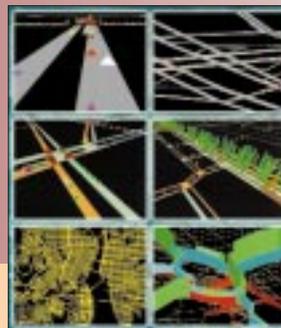


Transmission-corrected, gamma-ray emission computerized tomography shows the gamma-ray attenuating matrix material inside a 55-gallon drum.

CONTACT: THOMAS PRETTYMAN  
SAFEGUARDS SCIENCE AND TECHNOLOGY  
(505) 667-6449 • tprettyman@lanl.gov

### TRANSIMS: TRANSPORTATION ANALYSIS AND SIMULATION SYSTEM

Traffic congestion is at an all-time high in the United States and around the world, caused in part by an increasing number of motorists, vehicles and miles traveled. Such a situation causes longer delays and additional air quality problems in large cities, leading to lost productivity and added frustrations. Using the Transportation Analysis and Simulation System (TRANSIMS), transportation planners will understand better the effects of possible modifications to the transportation infrastructure, while accounting for traveler behavioral changes. The computer simulation system creates a virtual metropolitan region complete with a comprehensive representation of



An example of TRANSIMS micro-simulations of traffic interactions, freeway interchanges, traffic patterns, vehicle velocities, regional transportation networks and overlaid travel plans.

its population, traffic activities and transportation system. TRANSIMS helps scientists and planners calculate the potential effect of human behavior and resultant changes on energy consumption, traffic congestion, productivity and quality of life. Government decision-makers can save money and lives using TRANSIMS simulations to choose from among many alternatives to improve their transportation systems.

CONTACT: LARON SMITH  
TECHNOLOGY AND SAFETY  
ASSESSMENT DIVISION  
(505) 665-1286 • llsmith@lanl.gov



## DATELINE: LOS ALAMOS



**ON THE COVER:** Department of Energy laboratories won 21 of this year's R&D 100 Awards. Some of the winners include (clockwise from top left): a system that can detect chemical warfare agents in sealed containers, an innovative new barrier coating for flat panel displays, a dosimeter for food products undergoing cold pasteurization, a high-performance cement that can extend the life of geothermal wells, tiny metal particles that can enhance the effectiveness of rocket fuels and improve lubricants and (center) a revolutionary approach to materials research.

A MONTHLY PUBLICATION OF

LOS ALAMOS NATIONAL LABORATORY

### IN THIS ISSUE:

SCIENCE IN THE  
NATIONAL INTEREST  
PAGE 2

ADVANCED  
NONDESTRUCTIVE  
EVALUATION SYSTEM  
PAGE 8

ELECTROEXPLODED  
METAL NANOPARTICLES  
PAGE 10

17 OUTSTANDING  
RESEARCH EFFORTS  
PAGE 12

Dateline: Los Alamos is available  
on the World Wide Web:  
<http://www.lanl.gov/worldview/news/dateline/>



## DATELINE LOS ALAMOS

A MONTHLY PUBLICATION OF THE  
PUBLIC AFFAIRS OFFICE OF  
LOS ALAMOS NATIONAL LABORATORY

Nonprofit Organization  
U.S. Postage Paid  
Albuquerque, NM  
Permit No.532

LALP 00-1-9/10

**Los Alamos**  
NATIONAL LABORATORY